An NMR-based nanostructure switch for quantum logic

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We propose a nanostructure switch based on nuclear magnetic resonance (NMR) which offers reliable quantum gate operation, an essential ingredient for building a quantum computer. The nuclear resonance is controlled by the magic number transitions of a few-electron quantum dot in an external magnetic field.

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Quantum superposition and entanglement are currently being exploited to create powerful new computational algorithms in the growing field of quantum information processing. A major question for condensed matter physics is whether a solid-state quantum computer can ever be built. There are at least two basic requirements which must be met by any candidate designs: First is the ability to perform single quantum bit (qubit) rotations as well as two-qubit controlled operations, i.e. quantum gates. Second, the individual qubits should have a long decoherence time. Of utmost importance, therefore, is the identification of a solid-state system which can be used to represent the qubits.

Nuclei with spin $\frac{1}{2}$ are natural qubits for quantum information processing as compared to electrons [1], since they have a far longer decoherence time: indeed they have been used in bulk liquid NMR experiments to perform some basic quantum algorithms like those of Deutsch [2] and Grover [3]. Their exceptionally low decoherence rates allow implementation of quantum gates by applying a sequence of radio-frequency pulses. Nuclear spins have already been employed in some solid-state proposals, for example that of Kane [4] where a set of donor atoms (like P) is embedded in pure silicon. Here, the qubit is represented by the nuclear spin of the donor atom and single qubit and Controlled-Not (CNOT) operations might then be achieved between neighbor nuclei by attaching electric gates on top and between the donor atoms. Another proposal suggests controlling the hyperfine electron-nuclear interaction via the excitation of the electron gas in quantum Hall systems [5]. Both of these proposals, however, require the attachment of electrodes or gates to the sample in order to manipulate the nuclear spin qubit. Such electrodes are likely to have an invasive effect on the coherent evolution of the qubit, thereby destroying quantum information.

In this paper we present a new solid-state based proposal in which a nuclear spin is coupled, not with an electron gas, but with a reduced number of electrons in a quantum dot (QD). Our proposal avoids the complications associated with voltage gates or electron transport by providing an *all-optical* system. The nuclear resonance is controlled by exploiting the abrupt ground-state (so-called 'magic number') transitions which arise in a few-electron QD as a function of external magnetic field. The proposal was inspired by recent experimental results which demonstrated the optical detection of an NMR signal in both single QDs [6] and doped bulk semiconductors [7]. The experimental dots were formed by interface fluctuations in GaAs/GaAlAs quantum wells. The NMR signal from constituent Ga and As nuclei was optically detected via excitonic recombination, exploiting the hyperfine coupling between the electronic and nuclear systems. Hence the underlying nuclear spins in the QD can indeed be controlled with optical techniques, via the electron-nucleus coupling. In addition, the experimental results of Ashoori et al. [8] and others, have demonstrated that few electron (i.e. $N \geq 2$) dots can be prepared, and their magic number transitions measured as a function of magnetic field. The requirements for the present proposal are therefore compatible with current experimental capabilities.

Consider a silicon-based $N-$electron QD in which a ^{13}C impurity atom (nuclear spin $\frac{1}{2}$) is placed at the center [9]. Ordinary silicon (^{28}Si) has zero nuclear spin, hence it is possible to construct the QD such that no nuclear spins are present other than that carried by the carbon nucleus. Since carbon is an isoelectronic impurity in silicon, no Coulomb field is generated by this impurity. Hence the electronic structure of the bare QD is essentially unperturbed by the presence of the carbon atom. Suppose the quantum dot is quasi two-dimensional (2D) and contains $N = 2$ electrons. An external perpendicular magnetic field B is applied. The lateral confining potential in such quasi-2D QDs is typically parabolic to a good approximation: the electrons, with effective mass m^*, are confined to the $z = 0$ plane with lateral confinement $\frac{1}{2}m^*\omega_0^2 r^2$. Repulsion between electrons is modelled by an inverse-square interaction αr^{-2} which leads to the same ground-state physics as a bare Coulomb interaction r^{-1} [11,12]: moreover, such a non-Coulomb form may actually be more realistic due to the presence of image charges [13]. Any many-valley effects due to the band structure of silicon should be small and will be ignored.

In the effective mass approximation, the Hamiltonian is:

$$H = H_{2e} + C\sum_{\nu=1}^{2} \boldsymbol{I}\cdot\boldsymbol{S}_{\nu}\delta(\boldsymbol{r}_{\nu}) - \gamma_n B I_Z + \sum_{\nu=1}^{2}\gamma_e B S_{\nu,Z}, \quad (1)$$

where the electron-nucleus hyperfine interaction strength is given by $C = \frac{8\pi}{3}\gamma_e\gamma_n\hbar^2|\phi(z=0)|^2$, with $\phi(z=0)$ the single-electron wavefunction evaluated at the QD plane, γ_e (γ_n) is the electronic (nuclear) gyromagnetic ratio and $\boldsymbol{S}_{\nu}$ ($\boldsymbol{I}$) is the electron (nuclear) spin polarization. The electron location in the QD plane is denoted by the 2D vector $\boldsymbol{r}_{\nu}$. The first term represents the two-electron QD with a perpendicular $B-$field, the second is the Fermi contact hyperfine coupling of the nuclear spin with the electron spin, and the last two terms give the nuclear and the electron-spin Zeeman energies. Following Ref. [11], H_{2e} split up into commuting center-of-mass (CM) motion and relative motion (rel) contributions, for which exact eigenvalues and eigenvectors can be obtained analytically. The total energy is $E = E_{CM} + E_{rel} + E_{spin}$. The electron-electron interaction only affects E_{rel}.

The eigenstates of H can be labelled as $|I_Z; N, M; n, m; S, S_Z\rangle$, where N and M (n and m) are the Landau and angular momentum numbers for the CM (relative motion) coordinates; S and S_Z represent the total electron spin and its z-component, while I_Z represents the z-component of the carbon nuclear spin. Consider the two-electron system in its ground state, i.e. $N = M = 0$, $n = 0$; m determines the orbital symmetry while $S = 0, 1$ represents the singlet and triplet states respectively. The overall spin eigenstates have the form $|I_Z; S, S_Z\rangle_m$. For a given electron ground state orbital, the spin Hamiltonian matrix elements are:

$$\begin{aligned} H_S = \tfrac{C}{2}\sum_{\nu=1}^{2}\big\{&\delta_{I_Z,-}\delta_{I_{Z'},+}\langle S', S'_Z|\,\boldsymbol{S}_{\nu,-}\,|S, S_Z\rangle + \\ &\delta_{I_Z,+}\delta_{I_{Z'},-}\langle S', S'_Z|\,\boldsymbol{S}_{\nu,+}\,|S, S_Z\rangle + \\ &I_Z\delta_{I_Z I_{Z'}}\langle S', S'_Z|\,\boldsymbol{S}_{\nu,Z}\,|S, S_Z\rangle\big\}\langle m|\,\delta(\boldsymbol{r}_{\nu})\,|m\rangle + \\ &H_{Zeeman}, \end{aligned} \quad (2)$$

where H_{Zeeman} is the Zeeman term. In the presence of the $B-$field, the low-lying energy levels all have $n = 0$ and $m < 0$. The relative angular momentum m of the two-electron ground state jumps in value with increasing B (see Refs. [11] and [14]). The particular sequence of m values depends on the electron spin because of the overall antisymmetry of the two-electron wavefunction [14]. For example, only odd values of m arise if the $B-$field is sufficiently large for the spin wavefunction to be symmetric (the spatial wavefunction is then antisymmetric). These transitions, obtained analytically within our inverse-square model, yield the same sequence of transitions as for the Coulomb interaction. The electron-nucleus coupling depends on the wavefunction value at the nucleus and hence on m. The jumps in m will therefore cause jumps in the amount of hyperfine splitting in the nuclear spin of the carbon atom.

The nuclear spin$-$electron spin effective coupling affecting the resonance frequency $\omega_{_{NMR}}$ of the carbon nucleus is given by $\langle m|\,\delta(\boldsymbol{r}_{\nu})\,|m\rangle \equiv \Delta_{m,\nu}$, where

$$\Delta_{m,\nu} = \int d\boldsymbol{R}\int d\boldsymbol{r}\,\Psi^{*}_{2e}(\boldsymbol{R},\boldsymbol{r})\delta(\boldsymbol{r}_{\nu})\Psi_{2e}(\boldsymbol{R},\boldsymbol{r}) \quad . \quad (3)$$

Here $\Psi_{2e}(\mathbf{R},\mathbf{r}) = \xi_{N,M}(\mathbf{R})\zeta_{n,m}(\mathbf{r})$ where $\xi_{N,M}(\mathbf{R})$ ($\zeta_{n,m}(\mathbf{r})$) is the center-of-mass (relative) wavefunction [11]. A straightforward calculation gives $\Delta_{m,\nu} \equiv \Delta(m)$ where

$$\Delta(m) = \frac{1}{\pi l^2 2^{1+\mu_m}} \quad . \quad (4)$$

Here $l = \sqrt{\hbar/m^*\omega}$ is the effective magnetic length, the effective frequency is given by $\omega = \sqrt{\omega_c^2 + 4\omega_0^2}$, $\omega_c = eB/m^*$ is the cyclotron frequency. The term $\mu_m = \left(m^2 + \frac{\alpha/l_0^2}{\hbar\omega_0}\right)^{\frac{1}{2}}$ absorbs the effects of the electron-electron interaction and $l_0 = \sqrt{\hbar/m^*\omega_0}$ is the oscillator length. Hence, the effective spin Hamiltonian H_S (Eq. (2)) has the form

$$H_S = A(m)\left[(I_{+}S_{-} + I_{-}S_{+}) + 2I_{z}S_{z}\right] - \gamma_n B I_{z} + \gamma_e B S_{z} \quad (5)$$

where $A(m) = \frac{1}{2}C\Delta(m)$ represents a $B-$dependent hyperfine coupling. We note that the first term of the hyperfine interaction in Eq. (5) corresponds to the dynamic part responsible for nuclear-electron flip-flop spin transitions while the second term describes the static shift of the electronic and nuclear spin energy levels.

Electrons in the singlet state ($S = 0$) are uncoupled to the nucleus. In this case, the nuclear resonance frequency is given by the undoped-QD NMR signal $\omega_{_{NMR,0}} = \gamma_n B$. For electron triplet states, the nuclear resonance signal corresponds to a transition where the electron spin is unaffected by a radio-frequency excitation pulse whereas the nuclear spin experiences a flip. This occurs for the transition between states $|-; 1, -1\rangle$ and $|\Psi\rangle = c_1\,|+; 1, -1\rangle + c_2\,|-; 1, 0\rangle$. The coefficients c_1 and c_2 can be obtained analytically by diagonalizing the Hamiltonian given in Eq. (5) [15]. Hence

$$\begin{aligned} h\omega_{_{NMR}} = &\frac{3A(m)}{2} + \frac{1}{2}(\gamma_n - \gamma_e)B + \\ &\frac{1}{2}\left[\left[A(m) + (\gamma_n + \gamma_e)B\right]^2 + 8A^2(m)\right]^{\frac{1}{2}}. \end{aligned} \quad (6)$$

Since $\gamma_e >> \gamma_n$, $h\omega_{_{NMR}} \approx \gamma_n B + 2A(m)$ which illustrates the dependence of the NMR signal on the effective $B-$dependent hyperfine interaction.

Figure 1 shows the effective coupling $\Delta(m)$ between the two-electron gas and nucleus as a function of the ratio

between the cyclotron frequency and the harmonic oscillator frequency. (The CM is in its ground state). For silicon, $C/l_0^2 = 60MHz$. For B-field values where the electron ground state is a spin singlet (m even) no coupling is present. The strength of the effective coupling decreases as the $B-$field increases due to the larger spatial extension of the relative wavefunction at higher m values, i.e. the electron density at the centre of the dot becomes smaller. The $B-$field provides a very sensitive control parameter for controlling the electron-nucleus effective interaction. In particular, we note the large abrupt variation of $\Delta(m)$ for $\frac{\omega_c}{\omega_0} \approx 2.1$ where the electron ground state is performing a transition from a spin triplet state ($m = 1$) to a spin triplet state ($m = 3$). This ability to tune the electron-nucleus coupling underlies the present proposal for an NMR-based switch.

In the presence of infra-red (IR) radiation incident on the QD, the CM wavefunction will be altered since the CM motion absorbs IR radiation. (The relative motion remains unaffected in accordance with Kohn's theorem). This allows an additional method for externally controlling the nucleus-electron effective coupling, using optics. By considering the CM transition from the ground state $|N = 0, M = 0\rangle$ to the excited state $|N = 1, M = 1\rangle$, which becomes the strongest transition in high $B-$fields, we get the new spin-spin coupling term given by

$$\Delta_{\rm CM}(m) = \left(\frac{1+\mu_m}{2}\right)\Delta(m) \quad . \tag{7}$$

Hence the nuclear spin-electron spin coupling is renormalized by the factor $\frac{1+\mu_m}{2}$ in the presence of IR radiation. By changing the location of the impurity atom in the QD, the discontinuity strengths in Fig. 1 will be modified, since the coupling is affected by the density of probability of the CM wavefunction at the impurity site: future work will investigate the effect of placing impurities away from the QD center.

Figure 2 shows the relative variation of ω_{NMR} with respect to the undoped QD NMR signal, i.e. $\Delta\omega_{NMR} = \frac{\omega_{NMR}-\omega_{NMR,0}}{\omega_{NMR,0}}$ (solid line) as a function of the frequency ratio $\frac{\omega_c}{\omega_0}$. The jumps in the carbon nucleus resonance are abrupt, reaching 25% in the absence of IR radiation. This allows a rapid tuning on and off resonance of an incident radio-frequency pulse. The NMR signal in regions of spin-singlet states remains unaltered. The $B-$fields required to perform these jumps are relatively small (a few Tesla). Moreover, the nuclear spin is being controlled by radio-frequency pulses which are externally imposed, thereby offering a significant advantage over schemes which need to fabricate and control electrostatic gates near to the qubits, such as Refs. [4,5]. Illuminating the QD with IR light will shift the frequencies ω_{NMR} (see dotted line in Fig. 2) hence providing further all-optical control of the nuclear qubit. A crucial aspect of the present proposal is the capability to manipulate individual nuclear spins. All-optical NMR measurements in semiconductor nanostructures [6,7] together with local optical probe experiments are quickly approaching such a level of finesse.

The present proposal is not in principle limited to $N = 2$ electrons: generalizations [16–18] of the present angular momentum transitions arise for $N > 2$. It was pointed out recently [19] that the spin configurations in many-electron QDs could be explained in terms of *just* two-electron singlet and triplet states. Therefore, the present results may occur in QDs with $N > 2$. In addition, by employing QDs of different sizes, one could switch a subset of a QD array. Even if the QD array is irregular, one may still be able to perform the solid-state equivalent of the bulk/ensemble NMR computing recently reported in Ref. [20]: this again represents a potential advantage of the present scheme. Further advantages stem from the electrostatically neutral character of the impurity atom ^{13}C, and from the fact that the silicon nuclei surrounding it have no nuclear spin: the carbon nuclear spin state will be very effectively shielded from the environment and hence can be expected to have an even longer decoherence time than the (charged) donor nuclei in Ref. [4], thereby offering reliable quantum gate implementation.

Conditional quantum dynamics can be performed based on the selective driving of spin resonances of the two impurity nuclear qubits I_1, I_2 (spin $\frac{1}{2}$) in a system of two coupled QDs, separated by a distance d, each containing two electrons. The QDs do not need to be identical in size. The orthonormal computation basis of single qubits $\{|0\rangle, |1\rangle\}$ is represented by the spin up and down of the impurity nuclei. The Hamiltonian (1) must be modified: H_{2e} must include the effects of the intra-dot and inter-dot correlations between the two-body electron-electron interaction, and the effects of the electron and nuclear spins of the second QD must be included. Hence, we get an additional magic number transition as a function of $B-$field which can be used for selective switching between dots, i.e. since the ground state switches back and forth between pure and mixed states [21], the resonant frequency for transitions between the states $|0\rangle$, and $|1\rangle$ of one nuclear spin (target qubit) depends on the state of the other one (control qubit). In this way, such coupled QDs can be used to generate the conditional CNOT gate $\mathrm{CNOT}_{ij}(|\varphi_i\rangle|\varphi_j\rangle) \mapsto |\varphi_i\rangle|\varphi_i \oplus \varphi_j\rangle$ (where $\oplus$ denotes addition modulo 2 and the indices i and j refer to the control bit and the target bit) on the qubits $|\varphi_i\rangle$, and $|\varphi_j\rangle$. Single qubit rotations, e.g. the Hadamard transformation $H^T(|0\rangle) \mapsto \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and $H^T(|1\rangle) \mapsto \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ can be performed by rotating the single nuclear qubit via the application of an appropriate $B-$field. Note that the presence or absence of an IR photon can also represent a qubit: hence the present single QD system in an IR

cavity can also be used to perform two qubit gates as a result of the coupling.

In summary, we have proposed a solid-state qubit scheme which offers long decoherence times and reliable implementation of quantum gates. The fabrication requirements are compatible with current experimental capabilities. Being all-optical, rather than transport-based, the scheme avoids the need for electrical contacts and gates.

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Figure 1. Variation of the electron spin – nucleus spin effective coupling $\Delta(m)$ as a function of $\frac{\omega_c}{\omega_0}$; ω_c is proportional to the magnetic field and ω_0 represents the QD confining potential strength (see text). The center-of-mass motion remains in its ground state. The electron repulsion strength is given by $\frac{\alpha/l_0^2}{\hbar\omega_0} = 3.0$. The two-electron ground state undergoes transitions in the relative angular momentum m. The sequence, in terms of $|m|$ and the total electron spin S, is given by $(|m|, S) = \{(0,0),(1,1),(3,1),(5,1),...\}$.

Figure 2. Relative variation of the effective nuclear magnetic resonance frequency of the carbon impurity nucleus as a function of $\frac{\omega_c}{\omega_0}$. The electron repulsion parameter is the same as in Fig. 1. Solid line corresponds to center-of-mass in the ground state. Dotted line corresponds to center-of-mass in the first excited state after absorption of IR light.

Figure 1

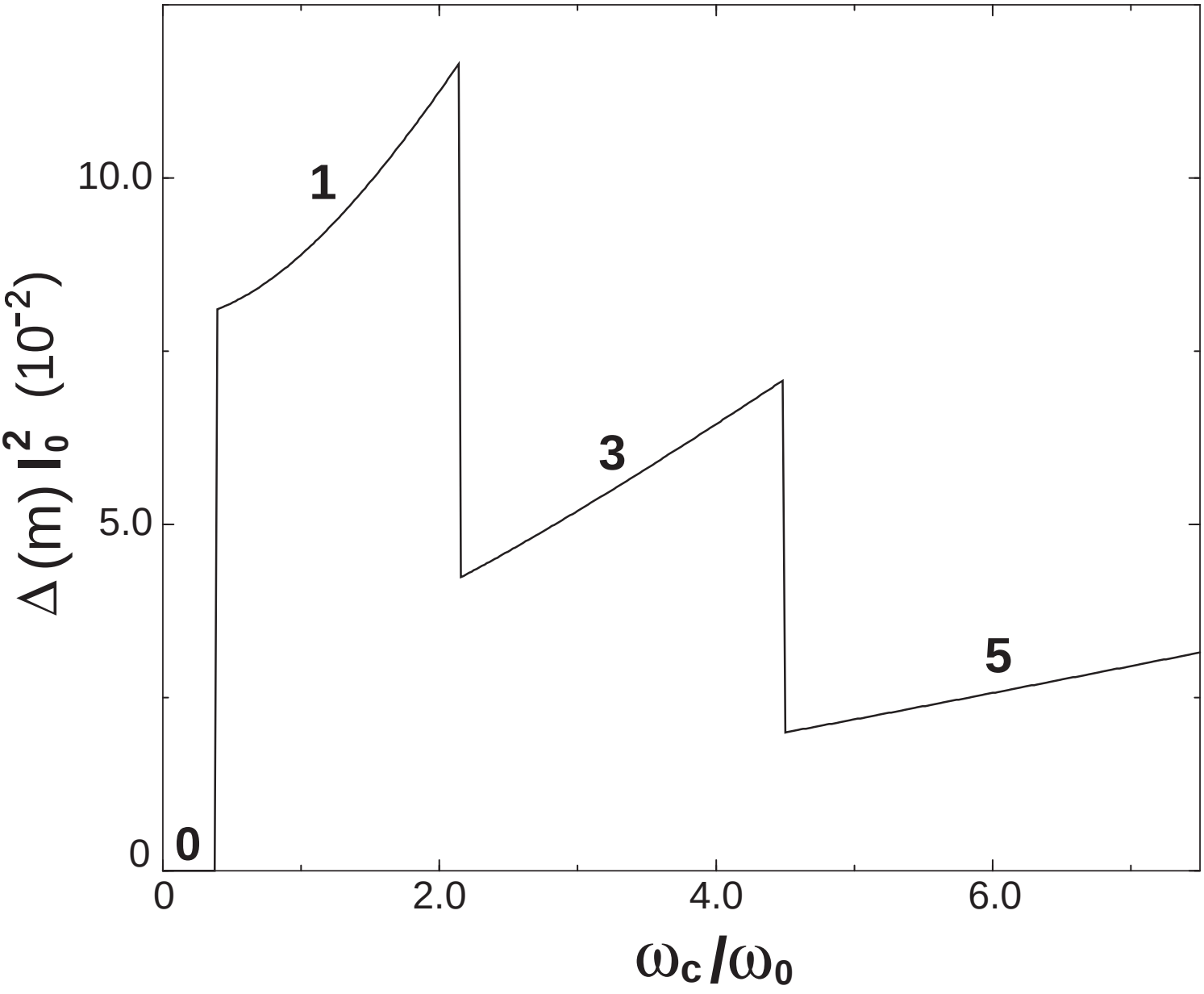

Figure 2